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In several recent theoretical studies, we have analyzed the local environment of deep-level defects through comparisons of theoretical and experimental hyperfine tensors. The principal hyperfine interactions sample the distribution of spin density near the center of the defect site, and are diagnostics of the local bonding conformation; the smaller hyperfine (superhyperfine) tensors, which are caused by couplings of the spin density with nuclei somewhat removed from the center of the defect, give valuable information about the embedding of the defect into the extended lattice of its solid-state host.

In the present article, we discuss the particular effect of dihedral angles on the second-neighbor superhyperfine interactions in broken-bond defects in silicon and $SiO_2$. This includes such defects centers as the $P_b$ center at the $Si/SiO_2$ interface, the E′ centers which occur in a-$SiO_2$ and quartz, and the D centers of hydrogenated amorphous silicon. The dihedral angle is found to affect the ability of the second-neighbor bonding atomic orbitals to couple to the defect hybrid and participate in the molecular orbital which carries the unpaired electron spin; the result is a significant dependence of second-neighbor superhyperfine splittings on the dihedral angle.

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# HYPERFINE AND SUPERHYPERFINE TENSORS AS PROBES OF THE LOCAL ENVIRONMENT OF DEEP-LEVEL DEFECT CENTERS*

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# HYPERFINE AND SUPERHYPERFINE TENSORS AS PROBES OF THE LOCAL ENVIRONMENT OF DEEP-LEVEL DEFECT CENTERS.*

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In several recent theoretical studies, we have analyzed the local environment of deep-level defects through comparisons of theoretical and experimental hyperfine tensors.[1,2] The principal hyperfine interactions sample the distribution of spin density near the center of the defect site, and are diagnostic of the local bonding conformation; the smaller hyperfine (superhyperfine) tensors, which are caused by couplings of the spin density with nuclei somewhat removed from the center of the defect, give valuable information about the embedding of the defect into the extended lattice of its solid-state host.

In the present article, we discuss the particular effect of dihedral angles on the second-neighbor superhyperfine interactions in broken-bond defects in silicon and $SiO_2$. This includes such defect centers as the $P_b$ center at the $Si/SiO_2$ interface, the E′ centers which occur in a-$SiO_2$ and quartz, and the D centers of hydrogenated amorphous silicon. The dihedral angle is found to affect the ability of the second-neighbor bonding atomic orbitals to couple to the defect hybrid and participate in the molecular orbital which carries the unpaired electron spin; the result is a significant dependence of second-neighbor superhyperfine splittings on the dihedral angle.

[1] M. Cook and C.T. White, *Phys. Rev. B* 38: 9674 (1988).
[2] M. Cook and C.T. White, *Semicond. Sci. Tech.* 4: 1012 (1989).

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